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Nanometric Modelization of Gas Structure, Multidimensional using COMSOL Software

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ABSTRACT

In structures with GaAs, which are the structures most used, because of their physical and electronic proprieties, nevertheless seems a compromise between the increase of doping and reduced mobility. The use of quantum hetero structures can overcome this limitation by creating a 2D carrier gas. Using the COMSOL software this work present three models: the first model computes the electronic states for the heterojunction AlGaAs/GaAs in 1D dimension, the second model computes the electronic states for the heterojunction AlGaAs/GaAs but in 2D dimension (nanowire) and the third model we permitted the study of this hetero junction (steep) wich inevitably involves the resolution of the system of equations Schrödinger-Poisson due to quantum effects that occur at the interface. The validity of this model can be effectuated with a comparison of our results with the result of different models developed in the literature of the related work, from this point of view the validity of our model is confirmed.

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1. INTRODUCTION

The emergence of III-V compound semiconductors has given a promising choice for channel material of future. These devices rely on the use of heterojunctions for their operation and high electron mobility transistors (HEMTs) are one of the most mature ones of the new generation of the III-V semiconductor transistors [1]. The heterojunctions in these devices are formed between semiconductors of differentcompositions and bandgaps, e.g. GaAs/AlGaAs and InGaAs/InP. These novel devices offer potential advantages in microwave. The High Electron Mobility Transistor (HEMT) is an important device for high speed, high frequency,digital circuits and microwave circuits with low noise applications. One of the properties of the family compound semiconductor III-V is indeed the probability of forming heterostructures with a good crystal interface (eg GaAs/AlAsGa) [1]. The gas formed by electrons accumulated at the interface of this hetero junction has two interesting physical properties: a two-dimensional character (The 2DEG electrons) and a very high mobility, especially at very low temperatures [1].

The HEMT transistor is essentially constituted of an AlGaAs/GaAs heterojunction, this heterojunction is considered as abrupt steep grace to very near stitch parameters and also grace to techniques of growth used for the fabrication of this heterojunction [2], [3]. The study of this heterojunction passes inevitable by the resolution of the system of Poisson Schrdinger equations [3], this system globally no linear doesn't have an analytic solution what gives back necessary a numeric resolution that can be effectuated by a self consist calculus. The 2DEG electrons attain greater energy and become hot with the moderate or higher elec-tric field. There will be an energy separation between the sub-bands, and the high mobility electrons in the lower sub-band get the needed energy from the applied electric field to move into the lower energy adjacent sub-band. Higher initial mobility in the lower sub-band results in the faster decay in mobility with

the applied voltage [2]. Hence with the applied electric field, the electrons at different sub-bands get the needed energy to move from their initial state and to move into the next state. This process makes the generation and recombination rate much faster resulting in better conduction of the device [2].

Low-dimensional quantum systems have been the subject of numerous studies in the past two decades. This interest is fueled both by surprising discoveries from the point of view of the physics of the condensed matter but also by the strong stake of manufacturing of electronic components [1]-[3]. Indeed, the permanent reduction in the size of architectures in microelectronics requires in the long term to take into account the quantum phenomena which considerably modify the physic. A new generation of electronic devices including the HEMT transistor has been developed taking advantage of these quantum effects.

The simulation environment used is undoubtedly of paramount importance, since the reliability and accuracy of the results depend directly on it. Initially, we had been thinking about the possibilities of using MATLAB to run our simulations. There were several reasons for this consideration. First of all, MATLAB is a distinctively well- known programming language, and is one which is highly acclaimed in the scientific, engineering and the academic community as a whole. Most of the research work we had studied for the purpose of this paper was employed in MATLAB in one way or the other. Due to its massive popularity, code examples and tutorials were readily available online. The MATLAB environment can seamlessly manipulate matrices and also came in with a command-line interface, thus making it a suitable tool for implementing numerical techniques, such as the Finite Difference Method. However, simulating in MATLAB meant designing and coding every aspect of the system from scratch, and we felt that this was somewhat of a repetitive process [4]. We were looking for a simulation environment that would allow us to get started right away, and with minimal effort. Although we were looking for simplicity and ease of use, we were, in no way, ready to compromise performance and accurate approximations to simulated results.

Taking the above factors into consideration, the second simulation environment we planned to resort to was SILVACO®. At the first glance, SILVACO seemed to overcome the limitations MATLAB exhibited. We had also dug up many research papers where SILVACO was employed to simulate semi-classical electrostatics simulations. However, we found the environment to be rather cumbersome and not user-friendly at all. On top of that, tutorials, documentations or any other resources on SILVACO were rarely found.

The third simulation environment we experimented with was COMSOL® Multiphysics®. COMSOL® Multiphysics® is a solution engine which solves partial differential equations via the finite element method (FEM) for a particular simulation [4]. This is the environment we finally settled for, and the reasons are many-fold. Firstly, as the name "Multiphysics" suggests, COMSOL has the capability to run multiple physics modules for a single simulation, and also allows "coupling" between compatible physics interfaces. This was suitable, since our underlying mechanism was to employ a Schrodinger-Poisson coupled solver. Plus, COMSOL provided many physics interfaces and add-ons right out of the box. Moreover, COMSOL had a myriad of documentation, ranging from blog posts to full-fletched video tutorials. The documentation that came in with the software was highly informative as well. COMSOL also supports integration with various software such as Excel and MATLAB which is referred to as a "Livelink". While searching for existing research done in COMSOL, it was found that simulations and studies have been done to find the depletion-all-around operation of n-channel four gate field effect transistors via the Poisson-Schrodinger equation [5]. The study of this (steep) heterojunction inevitably passed through the resolution of the system of Schrödinger-Poisson equations due of the quantum effects that occur at the interface. This work is consacreated to a Nanometric modelisation of a quantum well that has for aim to solve the system of equation Poisson Schrödinger using COMSOL SOFTWARE.

2. PROBLEMATIC

The structure under investigate consists for a N-typeAlGaAs layer and a P-type GaAs buffer layer. The nanametric structure has been investigated by using COMSOL SOFTWARE in the effective mass approximation and the envelope wave function vanishes at the interface [5]-[10]. The potential at the interface of heterojunction verify simultaneously the equation of Schrödinger and of Poisson that is why we propose to solve with rigorous way the system of equation Poisson Schrödinger given by the following formula [11]-[13]:

$$\begin{cases} Es: \dfrac{-\hbar^2}{2m_e}\Delta\Psi^i(z)+V(z)\Psi^i(z)=E^i\Psi^i(z) \\ Ep: V(z)+\dfrac{\rho(z)}{\varepsilon}=0 \end{cases}$$

Δ : The Laplacien operatorme: effective mass of an electron
$\Psi^i(z)$: Wave function associated with energy level Ei
V(z): The potential
ħ: Planck ‘s constant
ρ(z): Density of free electron it is given by:

$$\rho(z) = \begin{cases} qN_D - q\sum n(E^i)\left|\Psi^i(z)\right|^2 \cdots in\ GaAsAl \\ -qN_A - q\sum n(E^i)\left|\Psi^i(z)\right|^2 \cdots in\ GaAs \end{cases}$$

q: Electron charge
qND and -qNA: Fixed charge
ND: Donors doping rate
NA: Acceptors doping rate

$q\sum n(E^i)\left|\Psi^i(z)\right|^2$: Mobiles carrier

n (Ei): Carrier density (to the energy level of i number) of electrons obtained by the Dirac Fermi distribution it is given by:

$$n(E^i) = (\frac{m_e k_B T}{\pi\hbar^2})\log\left(1+\exp\frac{E_F - E^i}{k_B T}\right)$$

EF: Energy level of Fermi
KB: Boltzman constant
T: Absolute temperature
i: Number of state bound possible

3. SIMULATION AND RESULTS

3.1. Structure

As shown in the Figure 1, The modeled heterojunction(1D or 2D)is composed of two materials GaAS et AlGaAs (where the rate of Al is set to 0.3 o) where the latter is located to the left of the heterojunction. The contact of these two materials (parametry of crystal lattice very close) allowed the creation of a potential well in the buffer layer; where the energy will be quantified in a sequence of discrete levels of energy. Figure 2 show the 2D geometry of AlGaAs/GaAs heterojinction.

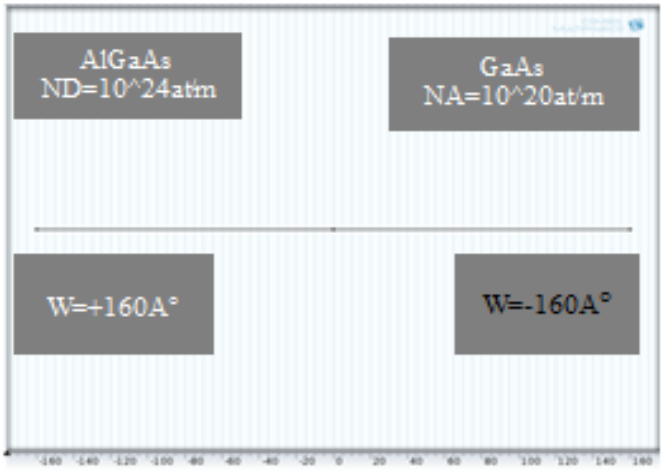

Figure 1. 1D geometry of AlGaAs/GaAs heterojinction

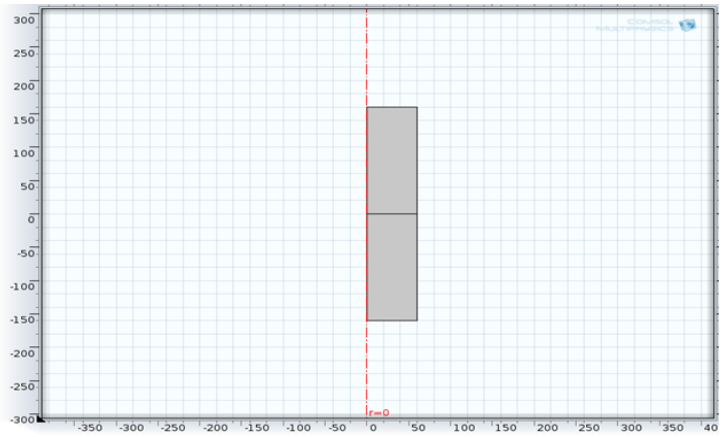

Figure 2. 2D geometry of AlGaAs/GaAs heterojinction

3.2. Physics

A Physics Interface in COMSOL provides all the domains, boundary conditions and the associated equations required for modeling a physical phenomenon or system. COMSOL also has the option for creating custom Physics interfaces. At the same time, some compatible physics interface can be coupled to one another. The two physics interface that we have used for our simulations – Coefficient Form PDE s interface and a Poisson equation interface. To computes the electronic states in 1Ddimention (quantumwell) or in 2Ddimention (nanowire), we have used the Coefficient Form PDE interface [14]. The model solves for an eigenvalue/Eigen function, for which you must input appropriate physical data and constants. Use electronvolts as the energy unit and nanometers as the length unit for the geometry.

To computes the potential energy and wave function for one band state, we have used tow physics the Coefficient Form PDE interface and Poisson equation. The model solves for an stationary step study with very precise initial parameters, for which we must input appropriate physical data and constants. The Finite Element Method (FEM) is employed by COMSOL behind the scene in order to find approximations to partial differential equations. Almost at all times, a simulation demands the solution of multiple partial differential equations.

In case of FEM, a single equation is approximated by a set of numerical model equations. This concept is better known as "discretization". Once the equation has a set of numerical components, each can be solved individually via numerical methods, and is then combined to yield the approximate solution to the partial differential equation. The finite element method can be observed to be employed extensively in the engineering community [15], primarily because of the freedom it provides while creating each element. The element distribution can be uniform or non-uniform, and hence can be manipulated to provide a required resolution. COMSOL provides multiple options for manipulating the element mesh distribution, ranging from normal to extra-fine to coarse.

3.3. Results

The wave function associated to bound state is illustrated on the Figure 3, Figure 4 and Figure 5 where we observed that the quantification of energy is located at some ten A in GaAs layer. Compered the model 1D and model 2D for heterojunction AlGaAs/GaAs, on the Table 1 we observed that the value of energy level have the same value for E_1,E_2,E_3 and different for E_4,E_5,E_6 because the model 1 computes the electronic states for a quantum well AlGaAs/GaAs (confinement 1D) and the model 2 computes the electronic states for a nanowire AlGaAs/GaAs (confinement 2D) [12]:

Table 1. The Six Lowest Bound States for the Heterojunctionalgaas/Gaas in 1D &2 D Simulation

Variable	Ei(1D)	Ei(2D)
1	0.019288	0.019299
2	0.077109	0.077149
3	0.173297	0.173368
4	0.3074416	0.251119
5	0.478072	0.307463
6	0.67174	0.308652

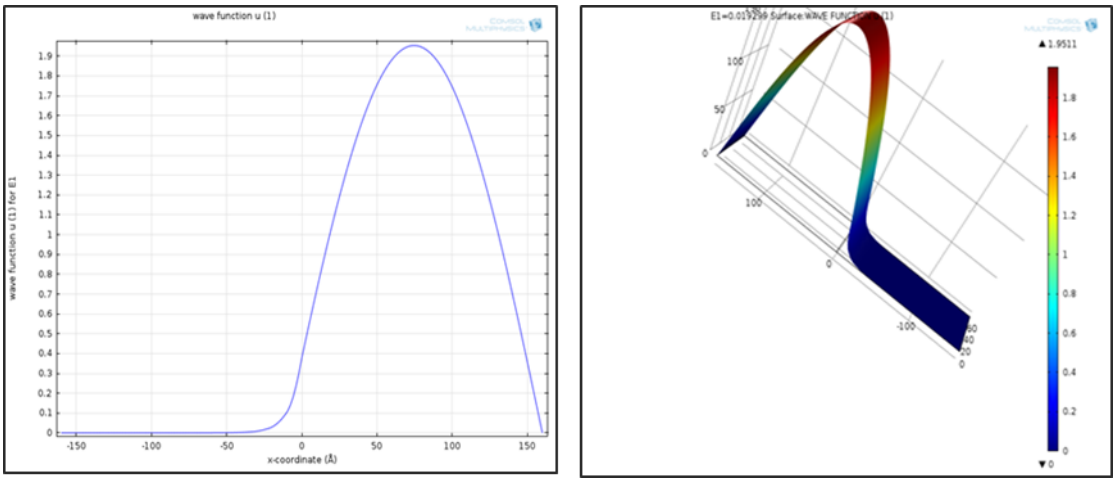

Figure 3. Wave function of E_1 for the heterojunction AlGaAs/GaAs in 1D&2D dimension

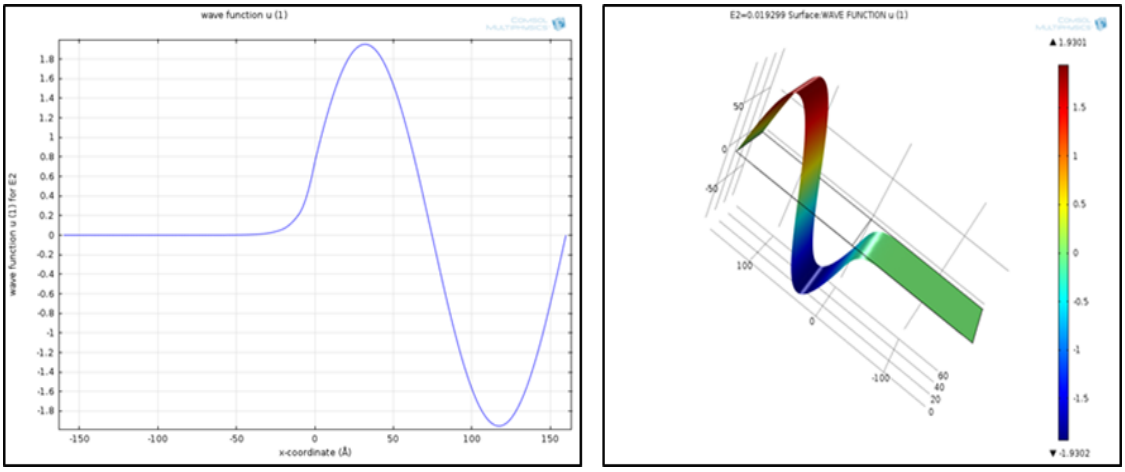

Figure 4. Wave function of E_2 for the heterojunction AlGaAs/GaAs in 1D&2D simulation

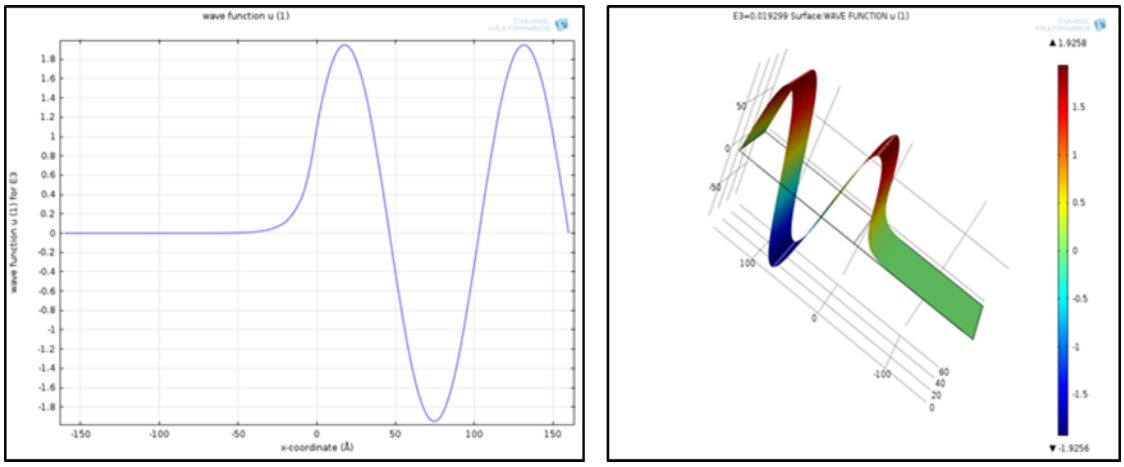

Figure 5. Wave function of E_3 for the heterojunction AlGaAs/GaAs in 1D&2D simulation

The Figure 6 represents potential well profile at the interface for unique bound state E=0.019288ev,

Figure 6 shows also the difference and the influence of the different numerical physical models on the shape of the potential well. Those different models proposed by the authors [7]-[10] are based on the self-consistent calculation which is based on an initial well (triangular initial potential), which gives the potential well the appearance of a peak. On the other hand, our model does not use any form given to the potential and/or wave function, it uses COMSOL multiphysics which gives the conduction bands the shape of a peak.

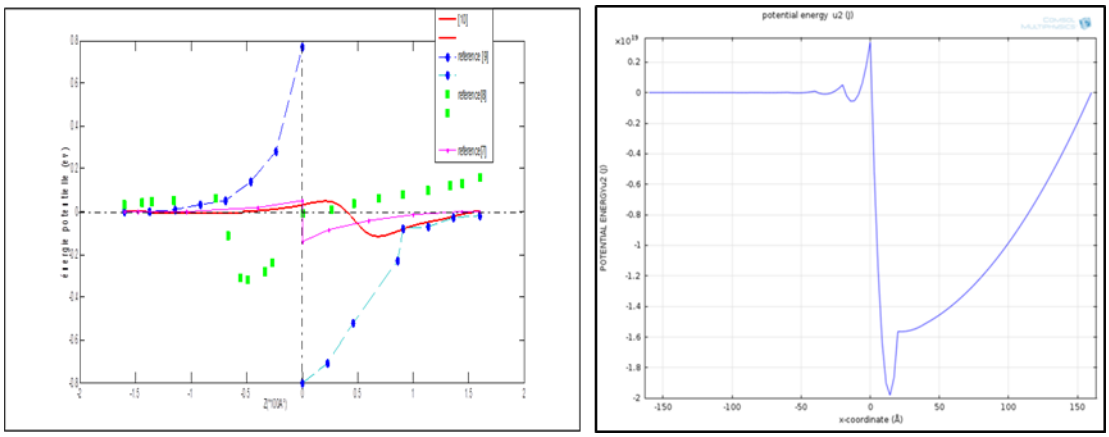

Figure 6. Potential energy for one band state compared with the literature

The wave function associated to one bound state is illustrated on the Figure 7 where we observed that the big probability to find electrons is also located at some ten A what implies that there is a penetration of the wave function in the potential well.

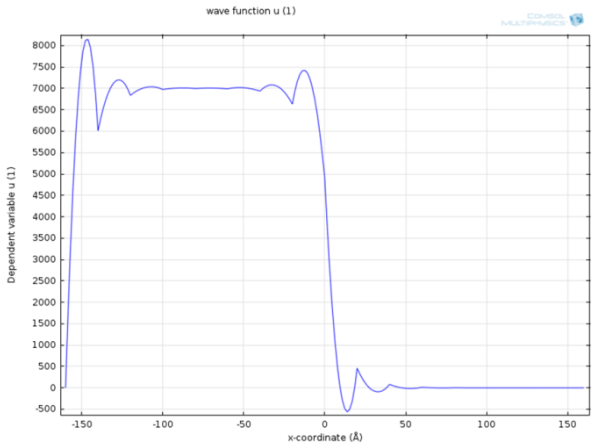

Figure 7. Wave function

4. CONCLUSION

Our work has as main objective the solution of Schrödinger-poisson system which is globally nonlinear in order to define the potential at the interface of a heterojunction GaAsAl/GaAs. We elaborate a calculus, using COMSOL MULTYPHYSICS software for a rigorous resolution. This modelisation that we have made can be applied to all other quantum heterojunction with inversion or accumulation layer.

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